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The Homogenization and Optimization of Thermoelectric Composites

Jiangyu Li
UNIVERSITY OF WASHINGTON

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Final Report

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14. ABSTRACT
We seek to understand the effective behavior of thermoelectric composites using rigorous homogenization technique in this project. In the last three years, our accomplishment includes: (1) rigorous analysis of thermoelectric field distribution and effective properties of layered thermoelectric structures, showing that their effective figure of merit is not bounded by the constituent phases, in contrast to the previous claim; (2) identification of condition for optimal conversion efficiency of layered structures, wherein the compatibility of optimal current density of individual phases is found to be the key; (3) extending the analysis of layered structures to the core-shell type of composites that are appropriate for many applications; (4) development of asymptotic analysis and homogenization of one-dimensional thermoelectric composites, for which closed-form solutions can be obtained; and (5) development of asymptotic analysis and homogenization of two- and three-dimensional thermoelectric composites, for which finite element simulations have been implemented. This set of theoretical and computational techniques can be used to guide the design and optimization of thermoelectric composites with optimal conversion efficiency.

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The Homogenization and Optimization of Thermoelectric Composites

Final Report

Jiangyu Li

Abstract

We seek to understand the effective behavior of thermoelectric composites using rigorous homogenization technique in this project. In the last three years, our accomplishment includes: (1) rigorous analysis of thermoelectric field distribution and effective properties of layered thermoelectric structures, showing that their effective figure of merit is not bounded by the constituent phases, in contrast to the previous claim; (2) identification of condition for optimal conversion efficiency of layered structures, wherein the compatibility of optimal current density of individual phases is found to be the key; (3) extending the analysis of layered structures to the core-shell type of composites that are appropriate for many applications; (4) development of asymptotic analysis and homogenization of one-dimensional thermoelectric composites, for which closed-form solutions can be obtained; and (5) development of asymptotic analysis and homogenization of two- and three-dimensional thermoelectric composites, for which finite element simulations have been implemented. This set of theoretical and computational techniques can be used to guide the design and optimization of thermoelectric composites with optimal conversion efficiency.

We seek to understand the effective behavior of thermoelectric composites using rigorous homogenization technique in this project. In the last three years, our accomplishment includes:

1. Rigorous analysis of thermoelectric field distribution and effective properties of layered thermoelectric structures, showing that their effective figure of merit is not bounded by the constituent phases, in contrast to the previous claim.

   In a well-known paper by Bergman and Levy published in Journal of Applied Physics in 1991, it was claimed that the effective figure of merit of a composite material is bounded by its constituent. This conclusion, however, was built on the linearized thermoelectric transport equations, which is not appropriate under large temperature difference for power generation operation. By using fully coupled nonlinear thermoelectric transport equation, we showed that this conclusion is incorrect, and a layered composite can achieve an effective figure of merit that is higher than its constituent phases. This work clarified a major misconception in the community. This paper was published in Journal of Applied Physics.

2. Identification of condition for optimal conversion efficiency of layered structures, wherein the compatibility of optimal current density of individual phases is found to be the key.

   In the course of analysis, we noted that the effective figure of merit of composites is actually ill-defined, due to nonlinearity involved. This is a well-known issue for nonlinear composites. As such, we analyzed the conversion efficiency of composite structure directly, and found that the effective conversion efficiency of a composite can be higher than its constituent. Even more important, we found that each constituent phase has its own optimal current density for high conversion efficiency, and in order for the composite to have overall optimal conversion efficiency, the optimal current density of each phase needs to be compatible with each other. Built on this observation, we also derived a new upper bound on the effective conversion efficiency of layered composites. This paper was published in Applied Physics Letters.

3. Extending the analysis of layered structures to the core-shell type of composites that are appropriate for many applications.

   We then extended our analysis of layered composite structure to radial geometry, with core-shell type of configuration. Such configuration is desirable for many applications involved in waste heat recovery, for example, for example exhaust heat from automobiles. The conclusion here is essentially similar to the layered structure. This paper was published in Acta Mechanica.

4. Development of asymptotic analysis and homogenization of one-dimensional thermoelectric composites, for which closed-form solutions can be obtained.

Here, we analyzed one-dimensional periodic thermoelectric composites using asymptotic analysis. Using separation of length scale and continuity of current density, we showed that zero-order term is the homogenized field distribution we are looking for, wherein the small scale fluctuation is smeared out when the size of heterogeneity approaches zero. Furthermore, we identified unit cell problems, on which the field distribution can be solved, and the governing equation for the homogenized field distribution can be obtained. These homogenized thermoelectric governing equations are more complicated than homogenous ones, but can still be solved analytically. This paper was published in Journal of Mechanics and Physics of Solids.

5. Development of asymptotic analysis and homogenization of two- and three-dimensional thermoelectric composites, for which finite element simulations have been implemented.

   The asymptotic analysis was extended to two- and three-dimensional periodic composites, wherein the current density is no longer a constant due to higher dimensionality. This complicates the analysis substantially, nevertheless, we were able to show that the zero-order term is still the homogenized solution, and we were able to identify the unit cell problem as well. The solution to the unit cell problem, however, has to be attacked numerically using finite element method, which we developed with our own code. This allows us to calculate the effective thermoelectric properties of three-dimensional composites with arbitrary microstructures. This work was published in another Journal of Mechanics and Physics of Solids paper.

In summary, we have developed a set of theoretical and computational techniques to analyze the effective behavior of thermoelectric composites, and they can be used to guide the design and optimization of thermoelectric composites with optimal conversion efficiency.

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Abstract

We seek to understand the effective behavior of thermoelectric composites using rigorous homogenization technique in this project. In the last three years, our accomplishment includes: (1) rigorous analysis of thermoelectric field distribution and effective properties of layered thermoelectric structures, showing that their effective figure of merit is not bounded by the constituent phases, in contrast to the previous claim; (2) identification of condition for optimal conversion efficiency of layered structures, wherein the compatibility of optimal current density of individual phases is found to be the key; (3) extending the analysis of layered structures to the core-shell type of composites that are appropriate for many applications; (4) development of asymptotic analysis and homogenization of one-dimensional thermoelectric composites, for which closed-form solutions can be obtained; and (5) development of asymptotic analysis and homogenization of two- and three-dimensional thermoelectric composites, for which finite element simulations have been implemented. This set of theoretical and computational techniques can be used to guide the design and optimization of thermoelectric composites with optimal conversion efficiency.

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Archival Publications (published) during reporting period:

Yang, Y., Xie, S. H., Ma, F. Y., & Li, J. Y. (2012). On the effective thermoelectric properties of layered heterogeneous medium. Journal of Applied Physics, 111(1), 013510.

Yang, Y., Ma, F. Y., Lei, C. H., Liu, Y. Y., & Li, J. Y. (2013). Is thermoelectric conversion efficiency of a composite bounded by its constituents?. Applied Physics Letters, 102(5), 053905.

Yang, Y., Ma, F. Y., Lei, C. H., Liu, Y. Y., & Li, J. Y. (2013). Nonlinear asymptotic homogenization and the effective behavior of layered thermoelectric composites. Journal of the Mechanics and Physics of Solids, 61(8), 1768-1783.

Yang, Y., Gao, C., & Li, J. (2014). The effective thermoelectric properties of core–shell composites. Acta Mechanica, 225(4-5), 1211-1222.

Yang, Y., Lei, C., Gao, C. F., & Li, J. (2015). Asymptotic homogenization of three-dimensional thermoelectric composites. Journal of the Mechanics and Physics of Solids, 76, 98-126.

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